

# Van Hove Singularity and D-Wave Pairing in Disordered Superconductors.

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We apply the coherent potential approximation (CPA) to a simple model for disordered superconductors with  $d$ -wave pairing. We demonstrate that whilst the effectiveness of an electronic Van Hove singularity to enhance the transition temperature  $T_c$  is reduced by disorder it is not eliminated. In fact we give a qualitative account of changes in the  $T_c$  vs. doping curve with increasing disorder and compare our results with experiments on the  $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2(\text{Cu}_{1-c}\text{Zn}_c)_3\text{O}_{7-\delta}$  alloys.

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According to a widely shared point of view the high transition temperature,  $T_c$ , of the superconducting cuprates is the consequence of a Van Hove singularity, in their normal state electronic structure, enhancing an otherwise unexceptional, that is to say weak, effective electron-electron attraction [1]. Clearly, if correct, this scenario would imply that relatively modest tinkering with such conventional mechanisms of pairing as electron-phonon interaction or spin-fluctuation could suffice to solve the central problem of high temperature superconductivity. This, conservative, view [2] is supported by two main observations. Firstly, most parameter free, first-principles, calculations find a Van Hove singularity near the Fermi energy  $\epsilon_F$  in these materials [3,4]. Secondly, the experimentally observed rise and fall of  $T_c$  with doping can be interpreted, very naturally, as due to  $\epsilon_F$  passing a Van Hove singularity. Of course, there are many objections to this, so called, Van Hove Scenario [1,5,6]. However, in the light of the emerging consensus that the Cooper pairs in these superconductors have  $d$ -like internal symmetry [7] two of these objections are particularly direct and damaging. The first one is that in the case of  $d$ -wave pairing the Van Hove mechanism is not effective. As it happens, this has been adequately answered by Newns et al. [8]. The other one concerns the particular sensitivity of  $d$ -wave pairing to disorder and will be addressed in the present letter.

In the case of  $s$ -wave superconductors the influence of scattering by defects, which do not break time reversal invariance, on  $T_c$  is governed by the Anderson's Theorem [9] and hence the disorder averaged density of states,  $\bar{n}(\epsilon)$ . Thus, the effect of disorder on the Van Hove Scenario is merely a question of smearing the structure in  $n(\epsilon)$  corresponding to the singularity. By contrast for  $d$ -wave superconductors there is no Anderson's Theorem and hence the role played by disorder is dramatically different. Not surprisingly, even without the complications introduced by Van Hove singularities the problem has been studied only recently and there are still many open questions [10–15]. In what follows, we generalize the Coherent Potential Approximation (CPA) for disordered superconductors [16] to the case of  $d$ -wave pairing. In general, the CPA is a significant improvement on beyond the self-consistent Born approximation (SBA) [17], currently in use for disordered  $d$ -wave superconductors. Elsewhere [18] we shall discuss in detail the formalism, differences between the CPA and the SBA, and various implications for experiments on high temperature superconductivity. However, in this letter we will focus our attention on investigating, for the first time, the viability of the Van Hove Scenario in  $d$ -wave superconductors in the presence of disorder.

Our arguments will be based on extended, negative  $U_{ij}$  Hubbard model on a lattice, whose sites are labelled by  $i$  and  $j$ , with random site energies  $\varepsilon_i$ . Moreover, we shall work in the Hartree–Fock–Gorkov approximation which implies that the usual one particle Green function matrix, in Nambu space, at the Matsubara 'frequency'  $\epsilon_n = \frac{\pi}{\beta}(2n+1)$  satisfies:

$$\sum_l \begin{pmatrix} (i\epsilon_n - \varepsilon_i + \mu)\delta_{il} + t_{il} & \Delta_{ij} \\ \Delta_{ij}^* & (i\epsilon_n + \varepsilon_i - \mu)\delta_{il} - t_{il} \end{pmatrix} \begin{pmatrix} G_{11}(l, j; \epsilon_n) & G_{12}(l, j; \epsilon_n) \\ G_{21}(l, j; \epsilon_n) & G_{22}(l, j; \epsilon_n) \end{pmatrix} = \delta_{ij} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (1)$$

where the hopping integrals  $t_{ij}$  and the pairing potentials  $\Delta_{ij}$  will be taken to be non zero only when the sites  $i$  and  $j$  are nearest neighbours,  $\mu$  is the chemical potential, and we shall often refer to the Greens function matrix as  $\underline{G}(i, j; \epsilon_n)$ . The above equations are completed by the self-consistency condition:

$$\Delta_{ij} = U_{ij} \frac{1}{\beta} \sum_n e^{i\epsilon_n \eta} G_{12}(i, j; \epsilon_n), \quad (2)$$

where  $U_{ij}$  is an attractive interaction energy between two electrons on nearest neighbour sites and  $\eta$  is a positive infinitesimal. To simplify matters we have assumed that the Hartree term can be absorbed into the hopping integral

$t_{ij}$  and dropped it from equation (1). As usual equations (1) and (2) are to be solved subject to the requirement on the chemical potential that

$$n = \frac{2}{\beta} \sum_n e^{i\epsilon_n \eta} G_{11}(i, i; \epsilon_n) , \quad (3)$$

where  $n$  is the number of electrons per unit cell.

Whilst, later, we shall refer to experiments on the substitutional alloys  $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2(\text{Cu}_{1-c}\text{Zn}_c)_3\text{O}_{7-\delta}$  [19] we do not wish to be very specific about the physical nature of the point defects represented by the site energies  $\epsilon_i$ . Indeed, we are content to provide a reliable analysis of the simplest possible non trivial model. Thus we take them to be independent random variables defined to have values  $\frac{1}{2}\delta$  and  $-\frac{1}{2}\delta$  with equal probability,  $\frac{1}{2}$ , on every site. As might be expected we shall be interested in the average of  $\underline{G}(i, j; \epsilon_n)$  over the above ensemble. To calculate  $\overline{\underline{G}}(i, j; \epsilon_n)$  we shall make use of the Coherent Potential Approximation which is well known to be the mean field theory of disorder for problems similar to the one at hand [20].

To define a tractable problem of interest we shall assume that the sites form a square lattice. Then for  $\epsilon_i = 0$  for all  $i$ , in the normal state, where  $\Delta_{ij} = 0$ , the spectrum features 4, well known, Van Hove singularities at  $\epsilon = 0$ , resulting in logarithmic divergence:  $n(\epsilon) \approx -\ln(\epsilon)$ . Below a certain temperature  $T_c$  there is a solution with  $\Delta_{ij} \neq 0$  and  $d$ -wave symmetry. As was pointed out by Newns et al. [8] in this model when  $n$  changes the Van Hove Scenario obtains as readily as in models where the symmetry of superconducting state is  $s$  type. That is to say  $T_c$  rises to a maximum at  $n = 1$  and then falls as  $n$  increases from  $n = 0$  to  $n = 2$  for a fixed interaction strength  $U_{ij}$ . As mentioned above, the technical question we shall answer in this letter is *what happens to this behaviour when the site energies are not zero but randomly  $\frac{1}{2}\delta$  or  $-\frac{1}{2}\delta$ ?*

Clearly, the relevant, generic, consequence of disorder is the smearing of structure in the density of states  $\overline{n}(\epsilon)$ . To gauge the extent of this in our model we calculated  $\overline{n}(\epsilon)$  using the standard CPA procedure [20]. The results, illustrating the smearing of the Van Hove singularities at  $\epsilon = 0$ , are shown in Fig. 1(a) for various values of the scattering strength  $\delta$ . In Fig.1(b) we also show the corresponding self energy  $\Sigma(\epsilon)$  which in CPA depends only on  $\epsilon$  but not on the wave vector  $\vec{k}$ . For our simple model  $\Sigma(\epsilon_n)$ , at the Matsubara frequency  $\epsilon_n$ , satisfies the following CPA equation [20]

$$\Sigma(\epsilon_n) = \left(\frac{1}{2}\delta - \Sigma(\epsilon_n)\right)\overline{G}(i, i; \epsilon_n)\left(\frac{1}{2}\delta + \Sigma(\epsilon_n)\right) . \quad (4)$$

It will be useful to note that in the weak scattering limit equation (4) reduces to the Self-consistent Born Approximation (SBA)

$$\Sigma^{SBA}(\epsilon_n) = \frac{\delta^2}{4}\overline{G}(i, i; \epsilon_n) \quad (5)$$

and hence on the real energy axis  $\text{Im}\Sigma(\epsilon) \sim n(\epsilon)$ . Interestingly, in the non-self-consistent Born approximation  $\text{Im}\Sigma(\epsilon)$  is logarithmically divergent at the van Hove singularity. In the disordered case one would expect such a singularity to be smeared out into a peak. Indeed the  $\delta = 0.6$  curve in Fig. 1(b) is fully consistent with this expectation. The other curves show the significant deviation, the split Van Hove singularity for instance, between CPA and SBA.

Let us now turn to the case where both superconductivity and disorder are present [16]. Although the full CPA program can be implemented for the problem defined by equations (1-3) and the specification of the site energy ensemble, it is convenient to make the approximation, valid when the coherence length  $\xi_0$  is much larger than the lattice spacing, that the pairing potential  $\Delta_{ij}$  does not fluctuate very much and replace it in equation (1) by its average value  $\overline{\Delta}_{ij}$  [21]. For conventional  $s$ -wave pairing this leads to the Anderson's Theorem [9] which means that the only effect of disorder is to replace the density of states in the gap equation by its ensemble average  $\overline{n}(\epsilon)$  [21]. Thus, in the Van Hove Scenario it is clear that the smearing of the Van Hove singularity in Fig. 1(a) implies a weakening of the Van Hove enhancement of  $T_c \sim \exp[-1/(U\overline{n}(\epsilon_F))]$ . The  $T_c$  at optimal doping will thus be significantly reduced by disorder, even for  $s$ -wave pairing.

As mentioned earlier the theory of disorder in  $d$ -wave superconductors turns out to be very different [10–15]. Nevertheless, the above simplification remains both valid and useful. In short we shall deploy the CPA to find  $\overline{\underline{G}}(i, j; \epsilon_n)$  for an averaged pairing potential  $\overline{\Delta}_{ij}$  (old) and recalculate  $\overline{\Delta}_{ij}$  (new) using equation (2) with  $G_{12}(i, j; \epsilon_n)$  replaced by  $\overline{G}_{12}(i, j; \epsilon_n)$  repeating the process until convergence. In this way self-consistency on the average is ensured.

To derive the basic CPA equations for disordered  $d$ -wave superconductors let us define the coherent Greens function  $\underline{\underline{G}}^c(i, j; \epsilon_n) \equiv \underline{\underline{G}}(i, j; \epsilon_n)$  by the equation:

$$\sum_l \begin{pmatrix} (i\epsilon_n + \mu - \Sigma_{11}(\epsilon_n))\delta_{il} + t_{il} & \bar{\Delta}_{il} \\ \bar{\Delta}_{il}^* & (i\epsilon_n - \mu - \Sigma_{22}(\epsilon_n))\delta_{il} - t_{il} \end{pmatrix} \underline{\underline{G}}^c(l, j; \epsilon_n) = \delta_{ij} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \quad (6)$$

where we did not introduce any off diagonal self-energies such as  $\Sigma_{12}(\epsilon_n)$  and  $\Sigma_{21}(\epsilon_n)$  because for the single site perturbations of our model they would turn out to be zero. The next step is to consider the scattering of the quasi-particles propagating according to  $G^c(i, j; \epsilon_n)$  by the defects described by the potentials:

$$\underline{\underline{V}}^\pm = \begin{pmatrix} \pm \frac{1}{2}\delta & 0 \\ 0 & \mp \frac{1}{2}\delta \end{pmatrix} - \begin{pmatrix} \Sigma_{11}(\epsilon_n) & 0 \\ 0 & \Sigma_{22}(\epsilon_n) \end{pmatrix} . \quad (7)$$

In a straightforward application of the CPA principles  $\underline{\underline{G}}(\epsilon_n)$  and therefore  $\underline{\underline{G}}^c(i, j; \epsilon_n)$  is determined by the condition that these defects do not scatter on the average. After some algebra this leads to the condition, similar to the one in equation (4), that:

$$\Sigma_{11}(\epsilon_n) = (\frac{1}{2}\delta - \Sigma_{11}(\epsilon_n))G_{11}^c(i, i; \epsilon_n)(\frac{1}{2}\delta + \Sigma_{11}(\epsilon_n)) . \quad (8)$$

We solved this equation numerically by iteration using the fact that  $G_{11}^c(i, j; \epsilon_n) = G_{11}^0(i, j; \tilde{\epsilon}_n, \tilde{\mu})$  where  $\underline{\underline{G}}^0$  is the solution of equation (1) with  $\varepsilon_i = 0$  for every  $i$ ,  $\Delta_{ij} = \bar{\Delta}_{ij}$  and the renormalized frequencies  $\tilde{\epsilon}_n$  and chemical potential  $\tilde{\mu}$  are given by

$$\tilde{\epsilon}_n = \epsilon_n - \text{Im}\Sigma_{11}(\epsilon_n) , \quad \tilde{\mu} = \mu + \text{Re}\Sigma_{11}(\epsilon_n) . \quad (9)$$

Note that equation (9) together with equation (8) constitutes a closed loop of relations which determine  $\tilde{\epsilon}_n$  or alternatively  $\Sigma_{11}(\epsilon_n)$ . Clearly, to solve this we need the Greens function matrix  $\underline{\underline{G}}^0(i, i; \epsilon_n)$ . This was obtained numerically by a very efficient recursion method [22].

To place above formulae in the context of previous work we note that in the weak scattering limit they reduce to those investigated in references [10,13–15] where  $\Sigma_{11}(\epsilon_n)$  was obtained by the SBA in equation (5). By contrast the CPA resums diagrams to all orders including some which have been investigated by Nersesyan et al. [12]. However, unlike them we find, analytically, that, for small  $\delta$ , near the Fermi energy  $\epsilon \approx 0$ ,  $n(\epsilon) \approx \frac{16\Delta}{\pi\delta^2} e^{\frac{-8\pi\Delta t}{\delta^2}} \neq 0$ , as in the earlier work of Gorkov and Kalugin [10].

In Fig. 2 we display our results for the evolution of the density of states  $n(\epsilon)$  and the self-energy  $\Sigma(\epsilon)$  with disorder, as described by  $\delta$ , at  $T = 0$ . As expected the overall effect of disorder is to fill in the v-shaped dip in the density of states near  $\epsilon_F$ . However, this process is rather intricate due to the competition between contributions in  $k$ -space from near the point where  $\Delta(\vec{k}) = 0$  and the Van Hove singularities at the saddle points. As a result, for small  $\delta$ , the strong scattering at the Van Hove singularity, evident in Fig. 1(b), is suppressed in the superconducting state by the dip, but eventually, for large  $\delta$ , disorder wins. Namely  $\Sigma_{11}(0)$  recovers and the gap is suppressed. Interestingly, the size of the ‘gap’ as measured by the distance between the two peaks in Fig. 2(a) remains roughly constant as the low energy dip is filled in. We have also performed finite temperature calculations relevant to tunnelling experiments [23], but we shall present these in a separate publication [18].

Finally we investigate the dependence of  $T_c$  on the band filling  $n$ . Our results for  $T_c$  vs.  $n$  are displayed in Fig. 3(a). For orientation we also calculated  $T_c$  as a function of  $n$  for an on site only, negative  $U$  Hubbard model with  $U_{ij} = -|U|\delta_{ij}$  and the same  $|U|$  and hopping integrals  $t_{ij}$  on the same lattice. The corresponding results are displayed in Fig. 3(b). Surprisingly, in spite of the delicate interaction between the Van Hove singularities and the very different behaviour of the quasiparticle spectra at low energies the two curves are largely similar. Hence, we may conclude that the Van Hove Scenario survives disorder almost as readily in  $d$ -wave superconductors as in the more conventional  $s$ -wave case. In support of the suggestion that this fact might have something to do with the superconducting cuprates we reproduce, in Fig. 4 the measurements of  $T_c$ , as a function of oxygen deficiency for various concentrations of Zn, made on  $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2(\text{Cu}_{1-y}\text{Zn}_y)_3\text{O}_{7-\delta}$  samples by Bernhard et al. [19]. Clearly if the Zn concentration is regarded of a measure of disorder and oxygen deficiency as that of doping these curves are very similar to our theoretical results in Fig 3(a). Thus our calculations support the interpretation of the experimental data by Bernhard et al. [19] as evidence for  $d$ -wave pairing.

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FIG. 1. Density of states  $N(E)$  (a) and self energies  $\Sigma(E)$  (b) for a normal state with various disorder strengths  $\delta$ .

FIG. 2. Density of states  $N(E)$  (a) and self energies  $\Sigma(E)$  (b) for a superconducting state with various disorder strengths  $\delta$ , calculated for  $|U| = 3.5t$  and  $n = 1$ .

FIG. 3. Critical temperature  $T_c$  vs. band filling  $n$  for  $d$  (a) and  $s$ -wave (b) superconductors and a number of disorder strengths  $\delta$  ( $|U| = 3.5t$ ).

FIG. 4.  $T_c$  as a function of oxygen deficiency  $\delta$  for  $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2(\text{Cu}_{1-y}\text{Zn}_y)_3\text{O}_{7-\delta}$  with  $y = 0$  (full squares),  $y = 0.02$  (triangles),  $y = 0.04$  (circles) and  $y = 0.06$  (stars) [19].













